On the monotonicity conjecture for the curvature of the Kubo-Mori metric *

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Abstract

The canonical correlation or Kubo-Mori scalar product on the state space of a finite quantum system is a natural generalization of the classical Fisher metric. This metric is induced by the von Neumann entropy or the relative entropy of the quantum mechanical states. An important conjecture of Petz that the scalar curvature of the state space with Kubo-Mori scalar product as Riemannian metric is monotone with respect to the majorisation relation of states: the scalar curvature is increases if one goes to more mixed states. We give an appropriate grouping for the summands in the expression for the scalar curvature. The conjecture will follows from the monotonicity of the summands. We prove the monotonicity for some of these summands and we give numerical evidences that the remaining terms are monotone too. Note that the real density matrices form a submanifold of the complex density matrices. We prove that if Petz's conjecture true for complex density matrices then it is true for real density matrices too.

1 Introduction

The state space of a finite quantum system can be endowed with a differentiable structure [10]. The canonical correlation defines a Riemannian structure on it. There is strong connection between the scalar curvature of this manifold at a given state and statistical distinguishability and uncertainty of the state [11]. Roughly speaking the scalar curvature measures the average statistical uncertainty. This idea comes from a series expansion of the volume of the geodesic ball. If D_0 is a given point in the state space and $B_r(D_0)$ is the geodesic ball with center D_0 and radius r then the volume of this ball is given by

$$V(B_r(D_0)) = \frac{\sqrt{\pi^n} r^n}{\Gamma\left(\frac{n}{2}+1\right)} \cdot \left(1 - \frac{\mathrm{Scal}(D_0)}{6(n+2)} \cdot r^2 + O(r^4)\right) \tag{1}$$

where $\mathrm{Scal}(D_0)$ is the scalar curvature at the point D_0 and n is the dimension of the manifold. There was given an explicit formula for the scalar curvature of these manifolds, for example in [3, 4, 7, 9]. Physically it is reasonable to expect that the most mixed states are less distinguishable from the neighboring ones than the less mixed states, for details see [10, 12]. It means mathematically that the scalar curvature of physically relevant Riemann structures should have monotonicity property in the sense that if D_1 is more mixed than D_2 then $\mathrm{Scal}(D_2)$ should be less then $\mathrm{Scal}(D_1)$. This was

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conjectured first by Petz [10] and it was verified for 2×2 matrices in [10]. There were some numerical simulations showing that the conjecture is true but no mathematical proof for that. The aim of the paper is to give an appropriate grouping for the summands in the expression for the scalar curvature and prove that some of these summands are monotone with respect to the majorisation.

The paper is organized as follows. In Section 2 definition, properties and equivalent forms of majorisation are given and the conjecture is formulated. In Section 3 the Kubo-Mori Riemannian inner product is defined and the curvature formula is given for real and complex density matrix spaces. In Section 4 we rewrite the scalar curvature formula as the sum of five terms. Four of them correspond with the conjecture as elementary, but brutal computations show. Further remarks and a lemma about the conjecture is presented as well. In Section 5 we prove that if the scalar curvature is monotone with respect to the majorisation on the space of complex density matrices then it is monotone on the space of real ones.

2 Majorisation

The state space of a finite quantum system is the set of positive semidefinite $n \times n$ matrices of trace 1. Such matrices are often called density matrices. Let $\mathcal{Q}_n^+$ denote the space of invertible density matrices. The state A is called majorised by the state B, denoted by $A \prec B$ if the following hold for their decreasingly ordered set of eigenvalues $(a_1, \ldots, a_n)$ and $(b_1, \ldots, b_n)$

$$\sum_{l=1}^{k} a_l \leq \sum_{l=1}^{k} b_l \tag{2}$$

for all $1 \leq k \leq n$. For any $(a_1, \ldots, a_n)$ eigenvalues of a density matrix

$$\left(\frac{1}{n}, \ldots, \frac{1}{n}\right) \prec (a_1, \ldots, a_n) \prec (1, 0, \ldots, 0).$$

The majorisation occurs naturally in various contexts. For example, in statistical quantum mechanics the relation $A \prec B$ is interpreted to mean that the state A describes a more mixed or a "more chaotic" state than B [1]. A linear map T on $\mathbb{R}^n$ a T-transform if there exists $0 \leq t \leq 1$ and indices k, l such that

$$T(x_1, \ldots, x_n) = (x_1, \ldots, x_{k-1}, tx_k + (1-t)x_l, x_{k+1}, \ldots, x_{l-1}, (1-t)x_k + tx_l, x_{l+1}, \ldots, x_n).$$

Note that if the density matrix A has eigenvalues $(a_1, \ldots, a_n)$ and the density matrix B has eigenvalues $T(a_1, \ldots, a_n)$ then $B \prec A$.

From every self-adjoint H operator and positive parameter β one can set a state

$$R_H(\beta) = \frac{e^{-\beta H}}{\operatorname{Tr} e^{-\beta H}} \tag{3}$$

which is called the Gibbs state at the inverse temperature β for the Hamiltonian H. One can check that if the difference $H_1 - H_2$ is a multiple of the identity then $R_{H_1}(\beta) = R_{H_2}(\beta)$. It is known that if $\beta_1 < \beta_2$ then $R_H(\beta_1) \prec R_H(\beta_2)$ [8]. This last result means that the states are more mixed at higher temperature.

Theorem 2.1. *Assume that we have two invertible states A and B with decreasingly ordered set of eigenvalues $(a_1, \ldots, a_n)$ and $(b_1, \ldots, b_n)$. The following are equivalent:*

1. *The state A is more mixed than B.*

2. *One can find a sequence $(C_z)_{z=1,\dots,d}$ between them such that for all $z=1,\dots,d$: $C_z \in \mathcal{Q}_n^+$,*

$$A = C_1 \prec C_2 \prec \cdots \prec C_d = B$$

   holds and the set of eigenvalues of C_z and C_{z-1} is the same except two elements.

3. *The set $(a_1,\dots,a_n)$ is obtained from $(b_1,\dots,b_n)$ by a finite number of T-transforms.*

4. *There is a sequence $(G_z)_{z=1,\dots,d}$ between them such that for all $z=1,\dots,d$: $G_z \in \mathcal{Q}_n^+$,*

$$A = G_1 \prec G_2 \prec \cdots \prec G_d = B$$

   holds and for all $i=1,\dots,d-1$ there exists a selfadjoint operator H_i and positive parameters $\beta_{1,i},\beta_{2,i}$ such that $G_i = R_{H_i}(\beta_{1,i})$ and $G_{i+1} = R_{H_i}(\beta_{2,i})$.

Proof. That (1) and (3) are equivalent can be found for example in [12]. The statement (2) is just the reformulation of (3). The implication (3) → (2) is trivial and easy to check that (2) → (3) implication holds too. □

After this introduction we can formulate correctly the Petz‘s conjecture [10].

Conjecture 2.1. *If $D_1 \prec D_2$ then $Scal(D_1) > Scal(D_2)$ where $Scal(D)$ denotes the scalar curvature of the state space induced by the canonical correlation inner product as Riemannian metric at the point D.*

3 Scalar curvature formula

Let $\mathcal{M}_n^+$ be the space of all complex self-adjoint positive definite $n \times n$ matrices and let $\mathcal{M}_n$ be the real vector space of all self-adjoint $n \times n$ matrices. The space $\mathcal{M}_n^+$ can be endowed with a differentiable structure [6] and the tangent space $T_D\mathcal{M}_n^+$ at $D \in \mathcal{M}_n^+$ can be identified with $\mathcal{M}_n$ [6]. One can consider the quantum mechanical state space $\mathcal{Q}_n^+$ as a Riemannian submanifold of $\mathcal{M}_n^+$ of codimension 1.

There is a very important functional on the space $\mathcal{M}_n^+$, namely the von Neumann entropy

$$S(D) = -\operatorname{Tr} D \log(D). \tag{4}$$

Since this functional is strictly concave [8, 12], the second derivative of the entropy

$$ddS : \mathcal{M}_n^+ \to \mathrm{LIN}(\mathcal{M}_n \times \mathcal{M}_n, \mathbb{R}) \quad D \mapsto \left((X,Y) \mapsto -\int_0^\infty \operatorname{Tr}\big((D+t)^{-1}X(D+t)^{-1}Y\big) \right) \tag{5}$$

is negative definite. The Riemannian metric which arises as the negative of the second derivative of the entropy

$$G_D(X,Y) = \int_0^\infty \operatorname{Tr}\big((D+t)^{-1}X(D+t)^{-1}Y\big)dt \tag{6}$$

is called Kubo-Mori metric. This scalar product is an important ingredient of linear response theory and often called the canonical correlation of X and Y.

Let us introduce this metric in a different way. Recall that Umegaki's relative entropy

$$S(D_1,D_2) = \operatorname{Tr} D_1(\log D_1 - \log D_2) \tag{7}$$

of density matrices measures the information between the corresponding states [8]. The partial derivatives of the relative entropy is the Kubo-Mori inner product:

$$\frac{\partial^2}{\partial t \partial s} \Big|_{t=s=0} S(D+tX, D+sY) = G_D(X,Y). \tag{8}$$

Let $D \in \mathcal{M}_n^+$ and choose a basis of $\mathbb{R}^n$ such that $D = \sum_{k=1}^n \lambda_k E_{kk}$ is diagonal, where $(E_{jk})_{j,k=1,\ldots,n}$ are the usual system of matrix units. Define the self-adjoint matrices

$$F_{kl} = E_{kl} + E_{lk} \quad H_{kl} = i\ E_{kl} - i\ E_{lk},$$

then the $(F_{kl})_{1\le k<l\le n}$, $(H_{kl})_{1\le k<l\le n}$ and $(F_{kk})_{1\le k\le n}$ vector system is a basis in $\mathcal{M}_n$. Let us define for positive numbers x,y,z the functions

$$m(x,y) := \int_0^\infty \frac{1}{(x+t)(y+t)} dt \qquad m(x,y,z) := \int_0^\infty \frac{1}{(x+t)(y+t)(z+t)} dt. \tag{9}$$

The scalar product of the basis vectors in the tangent space at the point D:

$$\begin{array}{ll} \text{for } 1\le i<j\le n,\ 1\le k<l\le n: & \begin{cases} G_D(H_{ij},H_{kl}) = G_D(F_{ij},F_{kl}) = \delta_{ik}\delta_{jl} 2m(\lambda_i,\lambda_j) \\ G_D(H_{ij},F_{kl}) = 0 \end{cases} \\ \text{for } 1\le i<j\le n,\ 1\le k\le n: & G_D(H_{ij},F_{kk}) = G(F_{ij},F_{kk}) = 0 \\ \text{for } 1\le i\le n,\ 1\le k\le n: & G_D(F_{ii},F_{kk}) = \delta_{ik} 4m(\lambda_i,\lambda_i) \end{array} \tag{10}$$

where $\delta_{ik}=1$ if $i=k$ else $\delta_{ik}=0$. We will use the following properties of the m functions: assume that x,y,z and μ are different positive numbers, then

$$\begin{array}{llll} m(x,y) = \dfrac{\log x - \log y}{x-y}, & m(x,y,z) = \dfrac{m(x,z)-m(y,z)}{x-y}, & m(x,x) = \dfrac{1}{x} & m(x,x,x) = \dfrac{1}{2x^2}, \\ m(x,y) = \dfrac{1}{\mu} m(\mu x,\mu y), & m(x,x,y) = \dfrac{m(x,y)-\frac{1}{x}}{x-y}, & m(x,y,z) = \dfrac{1}{\mu^2} m(\mu x,\mu y,\mu z). & \end{array} \tag{11}$$

The following identity will be used several times

$$\frac{1}{m(x,y)} \left(\frac{m(x,x,y)}{m(x,x)} + \frac{m(x,y,y)}{m(y,y)} \right) = 1. \tag{12}$$

Let us define two functions

$$\begin{aligned} \varphi(x,y,z) &= \frac{1}{2} \frac{m(x,y,z)^2}{m(x,y)m(y,z)m(z,x)} - \frac{m(y,y,x)m(y,y,z)}{m(y,x)m(y,y)m(y,z)}, \\ v(x,y) &= \frac{1}{2} \frac{m(x,x,y)^2}{m(x,y)^2 m(x,x)} - \frac{m(x,x,y)m(y,y,x)}{m(x,y)^2 m(y,y)}. \end{aligned} \tag{13}$$

From the definition and the identities (11) one can derive scaling properties

$$\varphi(\mu x,\mu y,\mu z) = \frac{1}{\mu}\varphi(x,y,z) \quad v(\mu x,\mu y) = \frac{1}{\mu} v(x,y). \tag{14}$$

The space $\mathcal{Q}_n^+$ is a one codimensional submanifold of $\mathcal{M}_n^+$. The tangent space of $\mathcal{Q}_n^+$ is the set of self-adjoint traceless matrices. The scalar curvature of this submanifold can be computed using the Gauss equation [2, 5].

The scalar curvature the space of complex density matrices at a given matrix D with eigenvalues $\lambda_1, \dots, \lambda_n$ is

$$\mathrm{Scal}(D) = \sum_{\substack{j,k,l=1 \\ |\{j,k,l\}|>1}}^{n} \varphi(\lambda_j, \lambda_k, \lambda_l), \tag{15}$$

where $|\{j,k,l\}| > 1$ means that the indices i, j and k are not equal [3], and that in the space of real density matrices is

$$\mathrm{Scal}_{\mathbb{R}}\, D = \frac{1}{4} \sum_{\substack{j,k,l=1 \\ |\{j,k,l\}|>1}}^{n} \varphi(\lambda_j, \lambda_k, \lambda_l) + \frac{1}{4} \sum_{k,l=1}^{n} v(\lambda_k, \lambda_l). \tag{16}$$

[7]. Note that the scalar curvature at a given point depends only on the eigenvalues of the density matrix.

4 About monotonicity of the scalar curvature

Using Theorem 2.1 the monotonicity conjecture will follows from the inequality

$$\mathrm{Scal}(A) = \mathrm{Scal}(C_1) \leq \mathrm{Scal}(C_2) \leq \cdots \leq \mathrm{Scal}(C_d) = \mathrm{Scal}(B).$$

Let A and B be two states, such that $A \prec B$ and the decreasingly ordered set of eigenvalues of A and B be the same except two elements. In this case their eigenvalues can be written in the form $(\lambda_1, \dots, a, \dots, b, \dots, \lambda_n)$ and $(\lambda_1, \dots, a - x, \dots, b + x, \dots, \lambda_n)$, where $x \leq \frac{a-b}{2}$.

If one computes the scalar curvature using equation (15) the summands can be grouped:

1. Summands where only a and b appear

$$\alpha(a,b) := 2\varphi(a,a,b) + 2\varphi(b,b,a) + \varphi(a,b,a) + \varphi(b,a,b). \tag{17}$$

2. Summands where a, b and another eigenvalue appears

$$\beta_{1,k}(a,b) := 2\varphi(a,a,\lambda_k) + 2\varphi(b,b,\lambda_k) + \varphi(a,\lambda_k,a) + \varphi(b,\lambda_k,b) \tag{18}$$

$$\beta_{2,k}(a,b) := 2\varphi(a,b,\lambda_k) + 2\varphi(b,a,\lambda_k) + \varphi(a,\lambda_k,b) + \varphi(b,\lambda_k,a). \tag{19}$$

3. Summands where a or b appear only once

$$\begin{aligned} \gamma_{kl}(a,b) :=& \varphi(a,\lambda_k,\lambda_l) + \varphi(b,\lambda_k,\lambda_l) + \varphi(\lambda_k,a,\lambda_l) \\ &+ \varphi(\lambda_k,b,\lambda_l) + \varphi(\lambda_k,\lambda_l,a) + \varphi(\lambda_k,\lambda_l,b). \end{aligned} \tag{20}$$

4. Summands without a and b

$$\delta_{jkl} := \varphi(\lambda_j, \lambda_k, \lambda_l).$$

After this grouping the curvature formula is

$$\mathrm{Scal}(D) = \alpha(a,b) + \sum_{k=1}^{n} \bigl(\beta_{1,k}(a,b) + \beta_{2,k}(a,b)\bigr) + \sum_{k,l=1}^{n} \gamma_{kl}(a,b) + \sum_{\substack{j,k,l=1 \\ |\{j,k,l\}|>1}}^{n} \delta_{jkl}. \tag{21}$$

One possible way to prove the monotonicity conjecture is to show that every summand in the previous formula is monotone with respect to the majorisation.

Dittmann used the symmetrization of function φ and the previous grouping of the scalar curvature in [3]. Numerical tests were confirmed by Dittmann about Petz's monotonicity conjecture and suggestive 3D-plots were given in [3].

Theorem 4.1. *Part α of the scalar curvature is monotone, that is for given $a > b$ positive numbers the function $\alpha(a-x, b+x)$ is strictly increasing in the variable $x \in \left[0, \frac{a-b}{2}\right]$.*

Proof. From the identities (11),(13) it follows, that

$$\varphi(a,b,a) + \varphi(b,a,b) = \frac{-1}{2(a+b)} \frac{1+b/a}{m(1,b/a)^2} \left(m(1,1,b/a)^2 + (b/a)m(b/a,b/a,1)^2 \right)$$

and

$$2\varphi(a,a,b) + 2\varphi(b,b,a) = \frac{-1}{a+b}(1+b/a)^2 \frac{m(1,1,b/a)m(b/a,b/a,1)}{n(1,b/a)^2}.$$

From these formulas and the special values of the functions m in (11) we obtain

$$\alpha(a-x, b+x) = \frac{-1}{a+b} \cdot \left(-\frac{1}{2}\frac{(1+c(x))^2}{(1-c(x))^2} + \frac{(1+c(x))(1+c(x)^2)}{c(x)(c(x)-1)\log c(x)} - \frac{1}{2}\frac{(1+c(x))^2}{c(x)\log^2 c(x)} \right),$$

where

$$c(x) = \frac{b+x}{a-x}.$$

Since the function $c(x)$ increasing, to prove the theorem it is enough to show that the function

$$\tau(c) = -\frac{1}{2}\frac{(1+c)^2}{(1-c)^2} + \frac{(1+c)(1+c^2)}{c(c-1)\log c} - \frac{1}{2}\frac{(1+c)^2}{c\log^2 c}$$

is decreasing on the interval I=$[0,1]$. To show that the function

$$\tau'(c) = \frac{(c+1)^2}{c^2\log^3 c} - \frac{(c+1)(3c^2-2c+3)}{c^2(c-1)\log^2 c} + \frac{c^4-2c^3-2c^2-2c+1}{c^2(c-1)^2\log c} + \frac{2c+2}{(c-1)^3}$$

is negative or equivalently the function

$$\tau_1(c) = (c-1)^3 \log^3 c \cdot \tau'(c)$$

is negative on the interval I, enough to prove that

(1) $\tau_1'(c) > 0$ on I and $\lim_{c\to 1} \tau_1(c) = 0$.

The limit can be easily checked and the first part will follow from the statement:

(2) $\tau_2(c) > 0$ on I and $\lim_{c\to 1} \tau_1'(c) = 0$,

where

$$\tau_2(c) = \frac{c^4}{(c-1)(c^2-c+1)(c^2+c+1)} \cdot \tau_1'(c).$$

Substituting τ_1' into the previous formula:

$$\tau_2(c) = 6\log^2 c + \frac{(c-1)(c+1)(c^2-12c+1)}{(c^2+c+1)(c^2-c+1)} \cdot \log c + \frac{(c+1)^2(c-1)^2}{2(c^2+c+1)^2(c^2-c+1)^2}.$$

The limit in the statement (2) again can be checked and the positivity of $\tau_2(c)$ will follow from the next statement

(3) $\tau_3(c) < 0$ on I and $\lim_{c\to 1} \tau_2(c) = 0$,

where

$$\tau_3(c) = c(c^2+c+1)^2(c^2-c+1)^2 \cdot \tau_2'(c).$$

Computation shows that

$$\begin{aligned}\tau_3(c) =& 2(6c^8+6c^7+13c^6-24c^5+22c^4-24c^3+13c^2+6c+6)\log c \\ &+ (c^8-12c^7+4c^6-4c^2+12c-1).\end{aligned}$$

The limit in the statement (3) again can be checked and the negativity of $\tau_3(c)$ will follow from the statement

(4) $\tau_3'(c) > 0$ on I and $\lim_{c\to 1} \tau_3(c) = 0$.

Easy to check that the limit condition fulfils in the previous statement, and the inequality is the following:

$$\begin{aligned}&4(24c^7+21c^6+39c^5-60c^4+44c^3-36c^2+13c+3)\log c \\ &+2\frac{(c-1)}{c}(10c^7-26c^6-c^5-25c^4-3c^3-27c^2-18c-6) \le 0.\end{aligned}$$

One can show that the coefficient of $\log c$ is strictly positive on I: The function $f_1(c) = c(100c^2 - 144c + 52)$ is positive on I. The function $f_2(c) = 7c^6 + 12c^5 - 14c^4 + 2$ has two stationary points on I: a local maximum at the origin and a local minimum at $c_0 = \frac{-15+\sqrt{813}}{21}$ and $f_2(c_0) > 0$. The coefficient of $\log c$ is

$$96c^7 + 6f_2(c) + f_1(c) + 36c^3(1-c)$$

which is positive on I.

Taking into account that the coefficients of $\log c$ is strictly positive on I one can rearrange the terms in the previous inequality:

$$q(c) = \log(c) + \frac{2(c-1)(10c^7-26c^6-c^5-25c^4-3c^3-27c^2-18c-6)}{c(96c^7+84c^6+156c^5-240c^4+176c^3-144c^2+52c+12)} \ge 0. \tag{22}$$

We will show this inequality in two steps.

1. $0 < c < \frac{1}{2}$: In this case let decrease the function $q(c)$ and show that the inequality

$$q^*(c) = \log(c) + \frac{3(c-1)(2c^7-1)}{c(24c^7+24c^6+44c^5-60c^4+44c^3-36c^2+13c+13)} \ge 0$$

holds. Since $q^*\left(\frac{1}{2}\right) > 0$, it is enough to show that $\frac{dq^*(c)}{dc} < 0$ if $0 < c < \frac{1}{2}$. This follows from the inequality

$$\begin{aligned}\frac{dq^*(c)}{dc} =& \frac{-1}{c^2(24c^7+24c^6+44c^5-60c^4+44c^3-36c^2+13c+3)^2} \cdot \\ &\cdot \Big(c^{12}(-576c^3-1440c^2-3216c+2112) + c^{10}(-2944c+1472) \\ &+ c^8(5296c^2-7700c+2640) + c^6(4800c^2-7292c+2508) \\ &+ c^3(1800c^3-568c^2-624c+241) + (550c^3-441c^2+69c+9)\Big),\end{aligned}$$

where $\frac{dq^*(c)}{dc}$ is the sum of six negative functions.

2. $\frac{1}{2} < c < 1$: Since $q(1) = 0$ enough to show that $q'(c) < 0$ if $\frac{1}{2} < c < 1$. Let us define the following function

$$\kappa(c) = -c^2(24c^7 + 24c^6 + 44c^5 - 60c^4 + 44c^3 - 36c^2 + 13c + 3)^2 \cdot q'(c).$$

The aim is to show that $\kappa(c)$ is positive if $\frac{1}{2} < c < 1$. Since

$$\kappa\left(\frac{1}{2}\right) \ , \ \kappa'\left(\frac{1}{2}\right) \ , \ \kappa^{(2)}\left(\frac{1}{2}\right) \ , \ \ldots \ , \ \kappa^{(9)}\left(\frac{1}{2}\right) > 0$$

enough to show that $\kappa^{(10)}(c) > 0$ if $\frac{1}{2} < c < 1$. This comes from the equality

$$\kappa^{(10)}(c) = 39916800(104832c^4 + 110292c^3 + 50688c^2 + 3963c + 1015).$$

□

Theorem 4.2. *Part $\beta_{1,k}$ of the scalar curvature is monotone, that is for given $1 > a > b$ positive numbers and eigenvalue $1 > \lambda_k > 0$ the function $\beta_{1,k}(a-x, b+x)$ is strictly increasing in the variable $x \in \left[0, \frac{a-b}{2}\right]$.*

Proof. From the identities (11) and (13) it follows, that

$$2\varphi(a, a, \lambda_k) + \varphi(a, \lambda_k, a) = \frac{1}{\lambda_k} \cdot \tau(a/\lambda_k),$$

where

$$\tau(c) = -\frac{2c-3}{2c\log^2 c} + \frac{1}{c(1-c)\log c} + \frac{c}{2(1-c)^2}.$$

From these equations one arrives at the expression

$$\beta_{1,k}(a-x, b+x) = \frac{1}{\lambda_k} \cdot \left(\tau\left(\frac{a-x}{\lambda_k}\right) + \tau\left(\frac{b+x}{\lambda_k}\right)\right).$$

This means that $\beta_{1,k}(a-x, b+x)$ is increasing if $\tau(\tilde{a} - \tilde{x}) + \tau(\tilde{b} + \tilde{x})$ is increasing on $[0, \frac{\tilde{a}+\tilde{b}}{2}]$, where $\tilde{a} = a/\lambda_k$, $\tilde{b} = b/\lambda_k$ and $\tilde{x} = x/\lambda_k$. To prove that

$$-\tau'(\tilde{a} - \tilde{x}) + \tau'(\tilde{b} + \tilde{x}) > 0$$

holds, which means that $\tau'(\tilde{x})$ decreasing, we will show that

$$\tau''(\tilde{x}) < 0.$$

We will do this in two steps: we show that the functions

$$\tau_1(c) = \frac{3-c}{4c\log^2 c} - \frac{1}{2c(c-1)\log c}, \quad \tau_2(c) = \frac{3-3c}{2c\log^2 c} - \frac{1}{c(c-1)\log c} + \frac{c}{(1-c)^2} \tag{23}$$

are concave, and we note that $\tau_1(c) + (1/2)\tau_2(c) = \tau(c)$.

In the concavity proof of $\tau_1(c)$ we work with the function

$$\tau^*(c) = -2c^3(c-1)^3\log^4 c \cdot \tau_1''(c)$$

that is

$$\begin{aligned}\tau^*(c) =& (6x^2 - 6x + 2)\log^3 x - (x-1)(3x-2)(x-3)\log^2 x \\ &+ (x-1)^2(x^2 - 10x + 11)\log x + 3(x-1)^3(x-3).\end{aligned}$$

To prove the concavity of $\tau_1(c)$ enough to show that $\tau^*(c)$ is negative if $c \in I$ and positive if $c > 1$.

Since $\lim_{c\to 1} \tau^*(c) = 0$ enough to show that $\tau^{*(1)}(c) > 0$.
Since $\lim_{c\to 1} \tau^{*(1)}(c) = 0$ enough to show that $\tau^{*(2)}(c)$ is negative if $c \in I$ and positive if $c > 1$.
Since $\lim_{c\to 1} \tau^{*(2)}(c) = 0$ enough to show that $\tau^{*(3)}(c) > 0$, or equivalently

$$\begin{aligned}\rho(c) =& c^3 \cdot \tau^{*(3)}(c) = (-18c^3 + 36c^2 - 18c + 12)\log^2 c\\ &+ (24c^4 - 138c^3 + 164c^2 + 34c - 12)\log c + (98c^4 - 276c^3 - 184c^2 - 4c - 2) > 0.\end{aligned}$$

Using the previous method the positivity of $\rho(c)$ comes from the positivity of the function $\rho^{(4)}(c)$ and the limits

$$\lim_{c\to 1} \rho^{(0)}(c) = \lim_{c\to 1} \rho^{(1)}(c) = \lim_{c\to 1} \rho^{(2)}(c) = \lim_{c\to 1} \rho^{(3)}(c) = 0.$$

The limits can be checked. The positivity of

$$\rho^{(4)}(c) = \frac{1}{c^4}\big(72(8c^4 - 3c^3 - 2c^2 + c - 2)\log c + 8(444c^4 - 153c^3 - 50c^2 + 4c + 42)\big)$$

comes from the series expansions of the log function. We will show that another expressions which are less then $\rho^{(4)}(c)$ are positive in two steps.

1. $c > 1$: It is known from the calculus that if $c > 1$ then

   $$\log c > 2\frac{c-1}{c+1}.$$

   Substituting $2\frac{c-1}{c+1}$ into $\rho^{(4)}(c)$ instead of $\log c$ one arrives at the expression

   $$\frac{1}{c^4(1+c)} \cdot \big(401c^5 + 185c^3(c^2 - 1) + 93c^4 + 8c(c-1) + 78\big)$$

   which is positive if $c > 1$.

2. $0 < c < 1$: The functions $f_1(c) = 8c^4 \log c + 1$, $f_2(c) = -(3c^3 + 2c^2 - c + 2)\log c$ and $f_3(c) = (444c^4 - 153c^3 - 50c^2 + 4c + 12)$ are positive on $[0,1]$. From this follows that

   $$\rho^{(4)} = \frac{1}{c^4} \cdot \big(72f_1(c) + 72f_2(c) + 8f_3(c) + 312\big) > 0 \qquad \text{if } 0 < c < 1.$$

We proved that the function $\tau_1(c)$ (was defined by (23)) is concave. In the concavity proof of $\tau_2(c)$ (was defined by (23)) we work with the function

$$\tau^*(c) = c^3(c-1)^4 \log^4 c \cdot \tau_2''(c),$$

that is

$$\begin{aligned}\tau^*(c) =& 2c^3(c+2)\log^4 c - 2(c-1)(3c^2 - 3c + 1)\log^3 c + (3c-2)(c-3)(c-1)^2\log^2 c\\ &- (3c^2 - 12c + 11)(c-1)^3 \log c - 9(c-1)^5.\end{aligned}$$

To prove the concavity of $\tau_2(c)$ enough to show that $\tau^*(c)$ is positive. Since one can check the following limits

$$\lim_{c\to 1} \tau^*(c) = \lim_{c\to 1} \tau^{*(1)}(c) = \cdots = \lim_{c\to 1} \tau^{*(5)}(c) = 0$$

enough to show that the function

$$\rho(c) = \frac{1}{c^2}\tau^{*(5)}(c) = 48(2c-1)\log^3 c + \frac{6}{c^3}(100c^4 - 11c^3 + 12c^2 + 12c + 12)\log^2 c - \frac{2}{c^3}(90c^5 - 246c^4 - 216c^3 - 62c^2 - 9c + 78)\log c - \frac{1}{c^3}(951c^5 - 642c^4 - 403c^3 - 36c^2 + 100c - 42)$$

is positive if $0 < c < 1$ and negative if $1 < c$. Using the previous methods again one can check that

$$\lim_{c\to 1}\rho(c) = \lim_{c\to 1}\rho'(c) = \lim_{c\to 1}\rho''(c) = 0.$$

This means that enough to show that the function

$$\frac{c^5}{2}\cdot\rho^{(2)}(c) = (144c^4 + 72c^3 + 72c^2 + 216c + 432)\log^2 c + (-180c^5 + 888c^4 - 78c^3 - 92c^2 - 306c - 1440)\log c - (1221c^5 - 1056c^4 + 282c^3 + 150c^2 + 273c - 870)$$

is positive if $0 < c < 1$ and negative if $1 < c$. Since

$$\lim_{c\to 1}\frac{c^5}{2}\cdot\rho^{(2)}(c) = 0$$

we will show that the function

$$\eta(c) = \frac{-1}{576c^3 + 216c^2 + 144c + 216}\cdot\frac{d}{dc}\left(\frac{c^5}{2}\cdot\rho^{(2)}(c)\right) \tag{24}$$

that is

$$\eta(c) = -\log^2 c + \frac{2(450c^5 - 1920c^4 + 45c^3 + 20c^2 - 63c - 432)}{c(576c^3 + 216c^2 + 144c + 216)}\cdot\log c + \frac{6285c^5 - 5112c^4 + 924c^3 + 392c^2 + 579c + 1440}{c(576c^3 + 216c^2 + 144c + 216)}$$

strictly positive.

We will show this inequality in two steps using an appropriate approximation of the log function.

1. $c > 1$: It is known that if $c > 1$ then $\sqrt{c} > \log c$. If one substitutes $-c$ into the previous formula instead of $-\log^2 c$ then one decreases the $\eta(c)$ function. We decrease again the function and multiplying by $1152c(11c^3 + 2c + 3)$ we show that

   $$-(91905c^4 - 9081c^3 - 9064c^2 + 2016c + 13824)\log c + \frac{(33c^3 + 6c + 9)(1855c^3 - 1776c^2 - 72)}{c}$$

   is positive. Since the coefficient of the $\log c$ is strictly negative if $c > 1$ enough to show that the function

   $$h(c) = -\log c + \frac{3(11c^3 + 2c + 3)(1855c^3 - 1776c^2 - 72)}{c(91905c^4 - 9081c^3 - 9064c^2 + 2016c + 13824)}$$

   is positive if $c > 1$. One can check that $h(1) = \frac{3}{800} > 0$ and

   $$h'(c) = \frac{864(87213719c^4 + 366253c^3 + 339642c^2 + 218160c + 10368) + c^4 q(c)}{c^2(91905c^4 - 9081c^3 9064c^2 + 2016c + 13824)^2}$$

where $q(c)$ is a polynom of c. To see that $h'(c)$ is positive if $1 < c$ enough to use the inequalities

$$q(1)\ ,\ q'(1)\ ,\ q^{(2)}(1)\ ,\ q^{(3)}(1) > 0$$

and the inequality

$$q^{(4)}(c) = 2376(852418875c^2 - 482743225c - 4909728) > 0 \qquad \text{if } 1 < c.$$

2. $0 < c < 1$: Since $\eta(1) > 0$ (η was defined by (24)) enough to show that

$$36c^2(8c^3 + 3c^2 + 2c + 3) \cdot \frac{d\eta(c)}{dc} < 0.$$

The previous expression is

$$(3600c^8 - 1908c^7 - 6876c^6 - 5552c^5 - 20058c^4 + 12888c^3 + 3210c^2 + 1080c + 1296) \cdot \log c$$
$$+ (28740c^8 + 4845c^7 + 2991c^6 + 22155c^5 - 35730c^4 - 25475c^3 - 7833c^2 - 3933c - 3456).$$

After increasing this expression and dividing by c^3 we will show that the function

$$-2c(954c^3 + 3438c^2 + 2776c + 10029) \cdot \log c + (28740c^5 + 4845c^4 + 2991c^3 + 22155c^2 - 35730c - 25475)$$

is still negative if $0 < c < 1$. Since the coefficient of $\log c$ is negative if $0 < c < 1$ we will show that the function

$$\eta^*(c) = \log c - \frac{28740c^5 + 4845c^4 + 2991c^3 + 22155c^2 - 35730c - 25475}{2c(954c^3 + 3438c^2 + 2776c + 10029)}$$

is positive if $0 < c < 1$. Since $\eta^*(1) > 0$ enough to show that

$$-2c^2(954c^3 + 3438c^2 + 2776c + 10029)^2 \cdot \frac{d\eta^*(c)}{dc}$$

is positive. Computing the previous expression we get

$$(472766109c^2 - 59724482c + 25548875) + a_3c^3 + a_4c^4 + \cdots + a_8c^8$$

where $a_3, a_4, \ldots, a_8 > 0$ and the first part is positive if $0 < c < 1$.

$\square$

The monotonicity of the function $\beta_{2,k}(a, b)$ means that for given positive numbers $1 > a > b$ and eigenvalue $1 > \lambda_k > 0$, the function $\beta_{2,k}(a-y, b+y)$ is strictly increasing in the variable $x \in \left[0, \frac{a-b}{2}\right]$.

Using the $\tilde{a} = \frac{a}{\lambda_k}$, $\tilde{b} = \frac{b}{\lambda_k}$ and $c = \frac{(a+b)}{2\lambda_k}$ notations the monotonicity means that the function $\beta_{2,k}(c + x, c - y)$ decreasing in the variable $x \in [0, c]$.

Let us define the following functions:

$$\phi_1(u) = \frac{1}{u \log u} + \frac{1}{1-u} \quad \phi_2(u) = \frac{1}{\log u} + \frac{1}{1-u}. \tag{25}$$

Using the equalities (11)

$$\lambda_k \cdot \beta_{2,k}(a, b) = 3w_\beta(x, c) + 2q_\beta(x, c) + 2r_\beta(x, c),$$

where

$$w_\beta(x,c) = \frac{m(c-x,c+x,1)^2}{m(c-x,c+x)m(c-x,1)m(c+x,1)}, \quad r_\beta(x,c) = -\frac{m(c-x,1,1)m(c+x,1,1)}{m(c-x,1)m(c+x,1)},$$
$$q_\beta(x,c) = \frac{-m(c-x,c-x,c+x)m(c-x,c-x,1)}{m(c-x,c-x)m(c-x,1)m(c-x,c+x)} - \frac{m(c+x,c+x,c-x)m(c+x,c+x,1)}{m(c+x,c+x)m(c+x,1)m(c-x,c+x)}.$$

These function can be computed explicitly:

$$w_\beta(x,c) = \frac{t_\beta(x,c)+t_\beta(-x,c)}{2}, \qquad \text{where} \quad t_\beta(x,c) = \frac{\frac{\log(c+x)}{\log(c-x)}\cdot\frac{c-x-1}{c+x-1}-1}{x(\log(x+c)-\log(x-c))},$$

$$q_\beta(x,c) = q_{1,\beta}(x,c)+q_{2,\beta}(x,c) \qquad \text{where} \quad \begin{cases} q_{1,\beta}(x,c) = \dfrac{\phi_1(c+x)-\phi_1(c-x)}{\log(x+c)-\log(x-c)}, \\ q_{2,\beta}(x,c) = \dfrac{\phi_2(c+x)}{x} + \frac{\phi_2(c-x)}{-x}, \end{cases}$$

$$r_\beta(x,c) = -\phi_2(c-x)\phi_2(c+x).$$

The monotonicity of the function $\beta_{2,k}$ comes from the inequality

$$\frac{d}{dx}\big(3w_\beta(x,c)+2q_\beta(x,c)+2r_\beta(x,c)\big) < 0.$$

This inequality is rather difficult to prove but it can be separated into four seemingly monotone part.

Theorem 4.3. *If for all positive parameters c the following conditions hold for all $x \in]0,c[$*

$$\begin{aligned} &\mathit{1:}\ \frac{d}{dx}\big(w_\beta(x,c)+q_\beta(x,c)\big) < 0 \qquad && \mathit{2:}\ \frac{d}{dx}\big(2w_\beta(x,c)+q_{1,\beta}(x,c)+r_\beta(x,c)\big) < 0 \\ &\mathit{3:}\ \frac{d}{dx}\big(q_{2,\beta}(x,c)\big) < 0 && \mathit{4:}\ \frac{d}{dx}\big(r_\beta(x,c)\big) < 0 \end{aligned} \tag{26}$$

then the $\beta_{2,k}$ part of the scalar curvature is monotone, that is for given $1 > a > b$ positive numbers and $1 > \lambda_k > 0$ eigenvalue the function $\beta_{1,k}(a-x,b+x)$ is strictly increasing in the variable $x \in \big[0, \frac{a-b}{2}\big]$.

Lemma 4.1. *The condition 4 fulfils in the previous theorem.*

Proof. The condition

$$\frac{d}{dx}\big(r_\beta(x,c)\big) < 0$$

is equivalent to the condition

$$\frac{\phi_2'(c+x)}{\phi_2(c+x)} > \frac{\phi_2'(c-x)}{\phi_2(c-x)},$$

where the function ϕ_2 was defined by (25), so enough to prove that

$$\left(\frac{\phi_2'(u)}{\phi_2(u)}\right)' > 0$$

or equivalently

$$\rho(u) = \phi_2(u)\phi_2''(u) - (\phi_2'(u))^2 > 0.$$

We will show that $\rho_*(u) = (1-u)^4\log^4 u \cdot \rho(u)$ is a positive function. Since

$$\rho_*(1) = \rho_*^{(1)}(1) = \rho_*^{(2)}(u) = \rho_*^{(3)}(1) = 0$$

enough to show that the function $\tau(u) = u^4 \cdot \rho_*^{(3)}(u)$ that is

$$\tau(u) = 2(-3u^3 - 6u^2 + u - 6)\log^2 u - 2(1-u)(2u^3 - 9u^2 - 3u + 2)\log u + 2(1-u)^2(6u^2 + 5u + 11)$$

is negative if $0 < u < 1$ and positive if $1 < u$. Since

$$\tau(1) = \tau^{(1)}(1) = \rho^{(2)}(1) = \tau^{(3)}(1) = \tau^{(4)}(1) = 0$$

enough to show that the function

$$\tau_*(u) = u^4 \cdot \tau^{(4)}(u)$$

that is

$$\tau_*(u) = (96u^4 - 72u^3 + 48u^2 + 8u + 144)\log u - 8(1-u)(61u^3 + 28u^2 + 28u + 30)$$

is increasing or equivalently

$$\tau_*^{(1)}(u) = (384u^3 - 216u^2 + 96u + 8)\log u \frac{8}{u}(256u^4 - 108u^3 + 6u^2 + 3u + 18) > 0.$$

After dividing the previous inequality with the coefficient of $\log u$ which is strictly positive if u is positive, the inequality is the following:

$$d(u) = \log u + \frac{16}{3} + \frac{18}{u} + \frac{1}{3} \cdot \frac{2484u^2 - 1284u + 655}{48u^3 - 27u^2 + 12u + 1} > 0. \tag{27}$$

We will show this inequality in three steps.

1. $0 < u < \frac{1}{2}$: Since $d\left(\frac{1}{2}\right) > 0$ enough to check that $d_*(u) = u^2(48u^3 - 27u^2 + 12u + 1)^2 \cdot d'(u)$ is negative if $0 < u < \frac{1}{2}$. Since $d_*(0) < 0$ enough to show that $d_*'(u) < 0$ and this inequality follows from the equation

   $$d_*'(u) = -u^5(25920 - 16128u) - u^2(-37245u^2 + 5400u^3 + 5000) - (5260u^2 - 2904u + 431),$$

   where $d_*'(u)$ is a sum of three negative terms.

2. $\frac{1}{2} < u < 1$: One can check that on this interval the function

   $$c(u) = \frac{1}{3} \cdot \frac{2484u^2 - 1284u + 655}{48u^3 - 27u^2 + 12u + 1}$$

   is concave hence

   $$c(u) > \frac{c(1) - c(1/2)}{1 - 1/2} \cdot (u - 1/2) + c(1/2) \qquad \text{if } \frac{1}{2} < u < 1.$$

   Substituting the right hand side of the previous inequality into the inequality (27)we get that

   $$\log(u) - \frac{113323}{2550} + \frac{18}{u} + \frac{13283}{425}u > 0.$$

   Let decrease the left hand side of the previous inequality and show that

   $$c_*(u) = \log u - 45 + \frac{18}{u} + 30u > 0 \qquad \text{if } \frac{1}{2} < u < 1.$$

   This function has only one stationary point which is a local minimum on this interval at $u_0 = \frac{\sqrt{2161}-1}{60}$ and $c_*(u_0) > 0$.

3. $1 < u$: Since $d(1) > 0$ (was defined by (27)) enough to show that $c(u) = u^2(48u^3 - 27u^2 + 12u + 1)^2 \cdot d'(u)$ is positive if $1 < u$. Since

$$c(1), c'(1), c^{(2)}(1), c^{(3)}(1), c^{(4)}(1) > 0$$

enough to show that $c^{(5)}(u) > 0$ if $1 < u$. This inequality follows from the equality

$$c^{(5)}(u) = 5806080u^2 - 3110400u + 893880.$$

$\square$

The conditions 1,2,3 in Theorem 4.3 hopefully can be proved similar way. The numerical evidences for previous theorem is the following:

There was chosen 10^4 parameter c uniformly from the interval $[0, 10^3]$ and for each chosen c the conditions 1,2,3 were numerically checked at 10^4 point uniformly from the interval $[0, c]$. This test can be view as a numerical evidence that the conditions 1,2,3 are valid.

The summand $\gamma_{kl}(a, b)$ in expression (21) can be computed using equalities (11), (13)

$$\gamma_{kl}(a,b) = \frac{3w(\tilde{a}, \tilde{\lambda}_k) + 3w(\tilde{b}, \tilde{\lambda}_k) + q(\tilde{a}, \tilde{\lambda}_k) + q(\tilde{b}, \tilde{\lambda}_k) + r(\tilde{a}, \tilde{\lambda}_k) + r(\tilde{a}, \tilde{\lambda}_k) + d(\tilde{a}, \tilde{\lambda}_k) + d(\tilde{a}, \tilde{\lambda}_k)}{\lambda_l},$$

where $\tilde{a} = \frac{a}{\lambda_l}$, $\tilde{b} = \frac{b}{\lambda_l}$, $\tilde{\lambda}_k = \frac{\lambda_k}{\lambda_l}$ and

$$w(x,c) = \frac{1}{(c-1)\log c}\left(\frac{\log c}{\log x - \log c} + \frac{1-c}{x-c}\right)\left(\frac{\log c}{\log x} + \frac{c-1}{1-x}\right), \qquad q(x,c) = \phi_1(c)\phi_2\left(\frac{x}{c}\right),$$
$$r(x,c) = \frac{-1}{x}\phi_2\left(\frac{c}{x}\right)\phi_2\left(\frac{1}{x}\right), \qquad d(x,c) = \phi_2(c)\phi_2(x).$$

The function $\phi_1(c)$ and $\phi_2(c)$ were defined by equation (25). The monotonicity of summand $\gamma_{kl}(a, b)$ means that the function $\gamma_{kl}(a - x, b + x)$ is increasing in the variable $x \in \left[0, \frac{a-b}{2}\right]$. This property follows from the inequality

$$\frac{d^2}{dx^2}\big(3w(x,c) + q(x,c) + d(x,c) + r(x,c)\big) < 0.$$

This inequality is rather difficult to prove but it seems that the left hand side of the previous inequality is the sum of two negative functions.

Theorem 4.4. *If for all c positive parameters the following conditions holds for all positive x*

$$1{:}\quad \frac{d^2}{dx^2}\big(2w(x,c) + d(x,c)\big) < 0 \qquad 2{:}\quad \frac{d^2}{dx^2}\big(w(x,c) + q(x,c) + r(x,c)\big) < 0$$

then the $\gamma_{k,l}$ part of the scalar curvature is monotone.

The conditions (1) and (2) in the previous theorem were tested numerically in the parameter space $x, c \in [0, 10^7]$, and the computation confirms the validity of the conditions.

Note that equation (21) not the only reasonable decomposition of the scalar curvature formula (15). There was tested many decomposition and the formula (21) seemed to be the most appropriate one. One can prove even more about summands in equation (21):

1. $\alpha(a,b)$ (defined by (17)):

   For given parameters $a > b > 0$ the functions

$$\begin{aligned}&\varphi(a-x, a-x, b+x) + \varphi(b+x, b+x, a-x),\\ &\varphi(a-x, b+x, a-x) + \varphi(b+x, a-x, b+x)\end{aligned}$$

   are strictly monotonously increasing if $x \in \left[0, \frac{a-b}{2}\right]$. From these follows Theorem (4.1).

2. $\beta_{1,k}(a,b)$ (defined by (18)):

   For given parameters $1 > a > b > 0$ and $1 > \lambda_k > 0$ the functions

$$\begin{aligned}&\varphi(a-x, a-x, \lambda_k) + \varphi(b+x, b+x, \lambda_k),\\ &\varphi(a-x, a-x, \lambda_k) + \varphi(b+x, b+x, \lambda_k) + \varphi(a-x, \lambda_k, a-x) + \varphi(b+x, \lambda_k, b+x)\end{aligned}$$

   are strictly monotonously increasing but the function

$$\varphi(a-x, \lambda_k, a-x) + \varphi(b+x, \lambda_k, b+x)$$

   is not increasing if $x \in \left[0, \frac{a-b}{2}\right]$.

3. $\beta_{2,k}(a,b)$ (defined by (19)):

   For given parameters $1 > a > b > 0$ and $1 > \lambda_k > 0$ the functions

$$\begin{aligned}&\varphi(a-x, b+x, \lambda_k) + \varphi(b+x, a-x, \lambda_k),\\ &\varphi(a-x, b+x, \lambda_k) + \varphi(b+x, a-x, \lambda_k) + \varphi(a-x, \lambda_k, b+x) + \varphi(b+x, \lambda_k, a-x)\end{aligned}$$

   seem to be (numerically tested) strictly monotonously increasing but the function

$$\varphi(a-x, \lambda_k, b+x) + \varphi(b+x, \lambda_k, a-x)$$

   is not increasing if $x \in \left[0, \frac{a-b}{2}\right]$.

4. $\gamma_{k,l}(a,b)$ (defined by (20)):

   For given parameters $1 > a > b > 0$ and $1 > \lambda_k, \lambda_l > 0$ the function

$$\varphi(\lambda_k, a-x, \lambda_l) + \varphi(\lambda_k, b+x, \lambda_l)$$

   seems to be (numerically tested) strictly monotonously increasing but the function

$$\varphi(a-x, \lambda_k, \lambda_l) + \varphi(b+x, \lambda_k, \lambda_l)$$

   is not increasing if $x \in \left[0, \frac{a-b}{2}\right]$.

   If one defines another symmetric function

$$\begin{aligned}\gamma^*_{kl}(a,b) =& \varphi(a, \lambda_k, \lambda_l) + \varphi(b, \lambda_k, \lambda_l) + \varphi(\lambda_k, a, \lambda_l)\\ &+ \varphi(\lambda_k, b, \lambda_l) + \varphi(\lambda_l, \lambda_k, a) + \varphi(\lambda_l, \lambda_k, b)\end{aligned}$$

   then the function $\gamma^*_{k,l}(a-x, b+x)$ will be not increasing if the ratio of λ_k and λ_l is large enough (~ 15000).

5 Scalar curvature on the real and complex state spaces

The real density matrices form a submanifold of the complex density matrices. The curvature tensors of a general submanifold can be very different from the curvature tensors of the manifold. For example one can think a circle (strictly positive scalar curvature) as submanifold of the plane (scalar curvature is 0). From this point of view one can reformulate Petz's conjecture for real density matrices. The question arises naturally: is there any connection between Petz's conjecture for real and complex matrices.

Theorem 5.1. *If the scalar curvature is monotone with respect to the majorisation on the space of complex density matrices then it is monotone on the space of real ones.*

Proof. From equations (15), (16) we get the equation

$$\mathrm{Scal}_{\mathbb{R}}(D) = \frac{1}{4}\,\mathrm{Scal}(D) + \frac{1}{4}\sum_{k,l=1}^{n} v(\lambda_k, \lambda_l),$$

where the function $v(\lambda_k, \lambda_l)$ was defined by (13). The monotonicity follows from the next two statements.

1. For every eigenvalues $\lambda_k > \lambda_l$ the function $v(\lambda_k - x, \lambda_l + x) + v(\lambda_l + x, \lambda_k - x)$ monotone increasing in the variable $x \in \left[0, \frac{\lambda_k - \lambda_l}{2}\right]$.

2. For every eigenvalues $\lambda_k > \lambda_l$ and λ_j the function $v(\lambda_k - x, \lambda_j) + v(\lambda_l + x, \lambda_j) + v(\lambda_j, \lambda_k - x) + v(\lambda_j, \lambda_l + x)$ monotone increasing in the variable $x \in \left[0, \frac{\lambda_k - \lambda_l}{2}\right]$.

Using equalities (11), (13) the function in the first statement can be written in the form

$$v(\lambda_k - x, \lambda_l + x) + v(\lambda_l + x, \lambda_k - x) = \frac{1}{\lambda_k + \lambda_l}\left[(1 + c(x))\kappa(c(x)) + \left(1 + \frac{1}{c(x)}\kappa\left(\frac{1}{c(x)}\right)\right)\right],$$

where

$$c(x) = \frac{\lambda_k - x}{\lambda_l + x}, \qquad \kappa(c) = \frac{3}{2c\log^2 c} - \frac{2c+1}{c(c-1)\log c} + \frac{c+2}{2(c-1)^2}. \tag{28}$$

Since the function $c(x)$ is decreasing enough to show that the function

$$d(c) = (1 + c)\kappa(c) + \left(1 + \frac{1}{c}\kappa\left(\frac{1}{c}\right)\right)$$

is decreasing if $c > 1$. This will follow from the negativity of the function

$$d_*(c) = (c-1)^3 \log^3 c \cdot d'(c).$$

Since

$$\lim_{c \to 1} d_*(c) = \lim_{c \to 1} d_*'(c) = 0$$

enough to show that

$$\tau(c) = \frac{1}{(1-c)(6c^4 + 18c^2 + 6)} \cdot d_*''(c) < 0 \qquad \text{if } 1 < c.$$

Since $\lim_{c \to 1} \tau(c) = 0$ enough to show that the function

$$\begin{aligned}\frac{3c(c^4 + 3c^2 + 1)^2}{(1-c)^2} \cdot \tau'(c) =& (6c^6 + 22c^5 + 59c^4 + 36c^3 + 59c^2 + 22c + 6)\log c \\ &+ \frac{5}{2}(1 - c^2)(c^4 + 6c^3 + 6c + 1)\end{aligned}$$

is positive. The coefficient of the $\log c$ is positive, so enough to show that

$$\tau_*(c) = \log c + \frac{5}{2}(1-c^2) \cdot \frac{c^4+6c^3+6c+1}{59c^2+22c+6} < 0 \quad \text{if } c > 1.$$

Since $\lim_{c\to 1} \tau_*(c) = 0$ enough to show that $\tau_*'(c)$ is positive and this follows from equation

$$\tau_*'(c) = \frac{a_0 + a_1 c + a_2 c^2 + \cdots + a_{12} c^{12}}{c(6c^6+22c^5+59c^4+36c^3+59c^2+22c+6)},$$

where $a_0, \ldots, a_{12}$ are strictly positive numbers.

This completes the proof of the first statement.

Using the equalities (11), (13) the function in the second statement can be written in the following form

$$\begin{aligned} v(\lambda_k - x, \lambda_j) + v(\lambda_l + x, \lambda_j) + v(\lambda_j, \lambda_k - x) + v(\lambda_j, \lambda_l + x) = \frac{1}{\lambda_j}\big(&\kappa(\tilde\lambda_k - \tilde x) + \kappa(\tilde\lambda_l + \tilde x) \\ &+ \rho(\tilde\lambda_k - \tilde x) + \rho(\tilde\lambda_l + \tilde x), \end{aligned}$$

where $\tilde\lambda_k = \frac{\lambda_k}{\lambda_j}$, $\tilde\lambda_l = \frac{\lambda_l}{\lambda_j}$, $\tilde x = \frac{x}{\lambda_j}$, the $\kappa(c)$ function was defined by (28) and

$$\rho(c) = \frac{3}{2\log^2 c} - \frac{c+2}{(c-1)\log c} + \frac{1+2c}{2(1-c)^2}.$$

Using the same arguments as in the proof of Theorem 4.2 enough to show that the function $\kappa(c)+\rho(c)$ is concave for all positive c. Let us define the function

$$d(c) = \frac{(c-1)^4 \log^4 c}{c+5} \cdot (\kappa''(c) + \rho''(c)).$$

To prove the second statement enough to show that $d(c) < 0$ for every positive c. Since

$$\lim_{c\to 1} d(c) = \lim_{c\to 1} d'(c) = \lim_{c\to 1} d^{(2)}(c) = \cdots = \lim_{c\to 1} d^{(6)}(c) = 0$$

enough to show that

$$\begin{aligned} \tau(c) = d^{(6)}(c) =& 1440\log^3 c - \frac{24}{c^5}(30c^6 - 211c^5 - 198c^4 + 207c^3 + 18c^2 + 54c + 90)\log^2 c \\ &+ \frac{8}{c^5}(1-c)(351c^5 + 1306c^4 - 29c^3 + 1120c^2 + 957c + 765)\log c \\ &+ \frac{4}{c^5}(1-c)^2(1249c^4 + 1132c^3 - 744c^2 - 872c - 705) < 0 \quad \text{if } 0 < c. \end{aligned} \tag{29}$$

Note that

$$\lim_{c\to 1} \tau(c) = \lim_{c\to 1} \tau'(c) = 0, \quad \lim_{c\to 1} (c^6\tau'(c))' < 0 \quad \text{and} \quad \tau(4), \tau'(4), (c^6\tau'(c))'(4) < 0.$$

To prove the inequality (29) for $0 < c < 1$ and $4 < c$ parameters enough to check that the function

$$\tau_*(c) = (c^6 \cdot \tau'(c))'' \tag{30}$$

is positive if $0 < c < 1$ and negative if $4 < c$. We will prove the inequality (29) in four steps.

1. $0 < c < \frac{1}{2}$: After decreasing the function $\tau_*(c)$ and dividing by c^2 one arrives at the inequality

$$\psi(c) = -78624\log^2 c + 96\frac{4483c^2+108}{c^3}\log c - 53008c + 194856 - \frac{76944}{c} - \frac{16208}{c^2} + \frac{56520}{c^4}.$$

   Since $\psi\left(\frac{1}{2}\right) = 0$ enough to show that

$$\begin{aligned}\psi_*(c) &= -\frac{c^4\psi'(c)}{157248c^3+430368c^2+31104} \\ &= \log c + \frac{16}{c}(3313c^5 - 31707c^3 - 2026c^2 - 648c + 14130) > 0.\end{aligned}$$

   Since $\psi_*\left(\frac{1}{2}\right) > 0$ enough to show that

$$p(c) = 3c^2(1638c^3 + 4483c^2 + 324)^2\psi_*'(c) < 0.$$

   The function $p(c)$ is a polynom and can be checked that $p(c) < 0$ if $0 < c < \frac{1}{2}$.

2. $\frac{1}{2} < c < 1$: After decreasing the function $\tau_*(c)$ (which was defined by (30)) one arrives at the inequality

$$-819c^2\log^2 c + \frac{4483c^2+108}{c}\log c - 553c^3 + 2029c^2 - 800c - 169 + \frac{588}{c^2} > 0 \quad \text{if } \frac{1}{2} < c < 1$$

   From the Taylor-expansion of the functions one can check that

$$\frac{4483c^2+108}{c}\log > a_0 + a_1(c-1/2) + a_2(c-1/2)^2, \quad -819c^2\log^2 c > b_0 + b_1(c-1/2),$$

   where

$$\begin{aligned} a_0 &= -\frac{4915\log 2}{2}, & a_1 &= 4915 - 4051\log 2, & a_2 &= 3187 - 864\log 2, \\ b_0 &= -\frac{819\log^2 2}{4}, & b_1 &= 819\log 2(1-\log 2). \end{aligned}$$

   After substituting the $\log c$ functions with the polynom of $(c-1/2)$ we get the following inequality

$$\frac{-1}{4c^2}(2212c^5 + \alpha_4c^4 + \alpha_3c^3 + \alpha_2c^2 - 2352) > 0$$

   where $\alpha_4 = 3456\log 2 - 20864$, $\alpha_3 = 3276\log^2 2 + 9472\log 2 - 3712$ and $\alpha_2 = -819\log^2 2 + 4230\log 2 + 7319$. One can check that the polynom in the parenthesis is strictly negative if $\frac{1}{2} < c < 1$.

3. $1 < c < 4$: Let increase the function $\tau(c)$ (defined by (23)): substitute $-2500(c-1)$ instead of

$$-\frac{24}{c^5}(30c^6 - 211c^5 - 198c^4 + 207c^3 + 18c^2 + 54c + 90)\log^2 c,$$

   and $-2000(c-1)^2$ instead of

$$\frac{8}{c^5}(1-c)(351c^5 + 1306c^4 - 29c^3 + 1120c^2 + 957c + 765)\log c$$

and $\frac{4}{c^5} \cdot (1-c)^2(1249c^4 + 1132c^3)$ instead of

$$\frac{4}{c^5}(1-c)^2(1249c^4 + 1132c^3 - 744c^2 - 872c - 705).$$

That these substitutions increases the function $\tau(c)$ can be check using the Taylor-expansion. The new inequality is

$$\tau_1(c) = 1440 \log^3 c + \frac{4(c-1)}{c^2} \cdot (500c^3 - 1124c^2 + 117c + 1132) < 0 \quad \text{if } 1 < c < 4.$$

Let increase the function $\tau_1(c)$:

$$\tau_2(c) = \tau_1(c) + 2000\frac{(c-1)(c-2)^2}{c^2}.$$

Since $\lim_{c \to 1} \tau_2(c) = 0$ to show that $\tau_2(c)$ is negative enough to check that $c\tau_2'(c) < 0$. Let increase the function $c\tau_2'(c) < 0$

$$\tau_3 = c\tau_2'(c) + 2000\left(c - \frac{3}{2}\right)^2 + 8(c-4)^2 - 72.$$

Since $\lim_{c \to 1} \tau_3(c) = 0$ to show that $\tau_3(c)$ is negative enough to check that

$$\tau_3'(c) = 8640 \log c + \frac{4(-996c^4 + 608c^3 + 2985c - 3472)}{c^2} < 0 \qquad \text{if } 1 < c < 4. \tag{31}$$

If $2 < c < 4$ then one can substitute $c - 1$ instead of $\log c$ and one can check that the inequality

$$\frac{-996c^4 + 2768c^3 - 2160c^2 + 2985c - 3472}{c^2} \quad \text{if } 2 < c < 4$$

holds. If $1 < c < 2$ then one can check the inequality (31) holds using the inequality

$$\frac{c-1}{c} + \frac{(c-1)^2}{2c^2} + \frac{(c-1)^3}{3c^3} + \frac{(c-1)^4}{4c^4} + \frac{(c-1)^5}{5c^5} + \frac{(c-1)^6}{c^6} > \log c \quad \text{if } 1 < c < 2.$$

4. $4 < c$: After increasing the function $\tau_*(c)$ (which was defined by (30)) one arrives at the inequality

$$(86400c^3 + 59616c + 2592)\log^2 c + \frac{48}{c}(-2985c^5 + 5840c^4 + 3126c^2 + 216)\log c + \frac{8}{c^2}(2184c^6 + 24357c^4 + 204c + 7065) < 0 \quad \text{if } 4 < c.$$

The coefficients of $\log^2 c$ and $\log c$ are positive and $c - 2 > \log^2 c$, $c - 2 > \log c$ if $4 < c$ therefore one way to increase the function is to substitute $c - 2$ instead of $\log^2 c$ and $\log c$. Then the new inequality is

$$c^4(5970c^3 - 27948c^2 + 30560c - 16855) + (17364c^3 - 216c^2 + 796c - 2355) > 0 \quad \text{if } 4 < c.$$

This inequality is holds since the left hand side is the sum of two positive functions on the $4 < c$ interval.

$\square$

6 Conclusions

We showed that Petz's monotonicity conjecture for the scalar curvature of the Kubo-Mori metric follows from more elementary inequalities. The key idea was to find a good grouping of summands in the expression of the scalar curvature. The proof of some inequality was given using elementary, but brutal computations. We proved that if Petz's conjecture holds for the manifold of complex density matrices then it is also true for the manifold of real ones.

The higher order derivatives of the summands of the scalar curvature play central role in these computations. The scalar curvature is a complicated expression of the Kubo-Mori metric, which can be derived from von Neumann entropy. It seems that these higher order derivatives (of the entropy function) responsible for the monotonicity of the scalar curvature. It would be good to find a proof for Petz's conjecture which is based only the easily computable properties of entropy function.

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